Research paper

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Orientations of Nonlocal Vibrational Modes from Combined Experimental and Theoretical Sum Frequency Spectroscopy

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Abstract. Inferring molecular orientations from vibrational sum frequency generation (SFG) spectra is challenging in polarization combinations that result in low signal intensities, or when the local point group symmetry approximation fails. While combining experiments with density functional theory (DFT) could overcome this problem, the scope of the combined method has yet to be established. Here, we assess its feasibility of determining the distributions of molecular orientations for one monobasic ester, two epoxides and three alcohols at the vapor/fused silica interface. We find that molecular orientations of nonlocal